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Structure-preserving Galerkin POD reduced-order modeling of Hamiltonian systems

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Highlights

- We propose a new structure-preserving reduced-order model for the Hamiltonian system.
- A rigorous *a priori* error estimate is presented for the structure-preserving ROMs.
- The approach modifies the traditional Galerkin projection-based POD-ROM.
- Motivated by the estimate, weighted gradient information of Hamiltonian is used.
- POD basis from shifted snapshots is used to improve the approximation to Hamiltonian.

Abstract

The proper orthogonal decomposition reduced-order model (POD-ROM) has been widely used as a computationally efficient surrogate model in large-scale numerical simulations of complex systems. However, when it is applied to a Hamiltonian system, a naive application of the POD method can destroy the Hamiltonian structure in the reduced-order model. In this paper, we develop a new reduced-order modeling approach for Hamiltonian systems, which modifies the Galerkin projection-based POD-ROM so that the appropriate Hamiltonian structure is preserved. Since the POD truncation can degrade the approximation of the Hamiltonian function, we propose to use a POD basis from shifted snapshots to improve the approximation to the Hamiltonian function. We further derive a rigorous *a priori* error estimate for the structure-preserving ROM and demonstrate its effectiveness in several numerical examples. This approach can be readily extended to dissipative Hamiltonian systems, port-Hamiltonian systems, etc.

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1. Introduction

Hamiltonian systems arise in many applications such as mechanics, meteorology and weather prediction, electromagnetism, and modeling of biological oscillators. Numerical simulations of such systems are usually large-scale and require long-time integration. Therefore, preserving intrinsic properties of the system is always used as an important criterion in the development of numerical schemes for such simulations. It is well known that numerical methods such as geometric integrator or structure-preserving algorithms are able to exactly preserve structural properties of Hamiltonian systems. For Hamiltonian ordinary differential equations (ODEs), development of structure-preserving schemes has achieved a remarkable success, such as the symplectic algorithms proposed in [1,2]. In the past two decades, various symplectic algorithms have been extended to Hamiltonian partial differential equations (PDEs) to preserve multi-symplectic conservation laws [3,4].

In recent years, there has been an increasing emphasis on constructing numerical methods to preserve certain invariant quantities such as the total energy of continuous dynamical systems. Various discrete gradient methods have been proposed in the literature, see for example [5,6]. The averaged vector field (AVF) method was proposed in [7] for canonical Hamiltonian systems, in which accurate computation of integrals is required. The method is extended in [8,9] to arbitrarily high order and non-canonical Hamiltonian systems. Based on the AVF method, a systematic energy-preserving or energy dissipation method is developed in [10]. The discrete variational derivative method is developed in [11] that inherits energy conservation or dissipation properties for a large class of PDEs. The method is further generalized in [12,13] to complex-valued nonlinear PDEs. The concept of the discrete variational derivative and a general framework for deriving integral-preserving numerical methods for PDEs were proposed in [14]. A class of new structure-preserving methods for multi-symplectic Hamiltonian PDEs was designed in [15].

Since many applications of Hamiltonian systems involve repeated, large-scale numerical simulations, reduced-order modeling can be employed to obtain an efficient surrogate model. One such model reduction technique is the proper orthogonal decomposition (POD) method, which has been successfully applied to many time-dependent, nonlinear PDEs [16–24] and the Hamiltonian dynamical system involved in the hybrid Monte Carlo sampling smoother [25]. The POD method is a data-driven approach, which extracts a few leading order, orthogonal basis functions from snapshots. By approximating the state variable in the subspace spanned by this basis set and combining with the Galerkin (or Petrov–Galerkin) methods, one can construct a low-dimensional dynamical system to approximate the original system. Because the dimension of the reduced-order model (ROM) is low, it is computationally inexpensive for numerical simulations. Although being successfully applied to many PDE models, the POD-ROM might be unstable for complex systems. To improve the stability, ROMs constructed on a modified projection subspace have been developed in [26] and the POD approaches based on a symmetry-based inner product or stabilizing projection have been introduced in [27–29] to preserve certain quantities such as the energy of compressible flows.

When a Hamiltonian system is considered, the Galerkin projection-based POD-ROM is not able to preserve desired physical quantities because the Hamiltonian structure of the original system may not be retained in the reduced dynamical system. This issue has been discussed recently and attempts have been made to address it. For example, structure-preserving interpolatory projection methods are developed in [30] to keep structures such as symmetry of linear dynamical systems. It is then extended to port-Hamiltonian systems via tangential rational interpolation in [31]. For port-Hamiltonian systems, structure-preserving Petrov–Galerkin reduced models are introduced in [32], in which the POD-based and $\mathcal{H}_2$-based projection subspaces are discussed. A combination of POD and $\mathcal{H}_2$ quasi-optimal selections of the subspace as well as a structure-preserving nonlinear model reduction via discrete empirical interpolation method (DEIM) is recently developed in [33]. A proper symplectic decomposition (PSD) approach based on the symplectic Galerkin projection is proposed in [34] for developing ROMs of the Hamiltonian PDEs with a symplectic structure. Three algorithms are designed to extract the PSD basis from snapshots computed. There are some other model reduction approaches that aim to preserve Lagrangian structures [35,36], where the Galerkin projection is carried out in the Euler–Lagrange equation, not the first-order state-space form.

In this paper, we consider Hamiltonian PDEs given in first-order differential equation(s), and adapt the Galerkin projection-based POD-ROM to preserve the appropriate Hamiltonian structure. Due to the POD truncation, there may exist discrepancies in the approximation of the Hamiltonian function between the new ROM and the full-order model (FOM). Thus, we introduce the POD basis from shifted snapshots to improve the reduced-order approximation.